12/20/04

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=> d l1
L1 HAS NO ANSWERS
L1                STR
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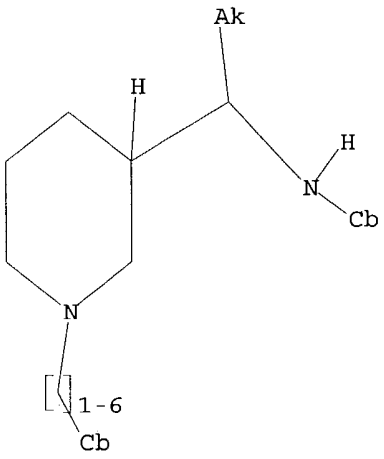


G1 H,Ak,Cb

G2 Cb,Ak

G3 H,Ph,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 14:15:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   5057 TO ITERATE

 19.8% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         96876 TO   105404
PROJECTED ANSWERS:                0 TO        0

L2             0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 14:15:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 101916 TO ITERATE

100.0% PROCESSED  101916 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.05

L3             0 SEA SSS FUL L1

=> file registry
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.84     156.05
```

12/20/04

FILE 'REGISTRY' ENTERED AT 14:16:26 ON 20 DEC 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

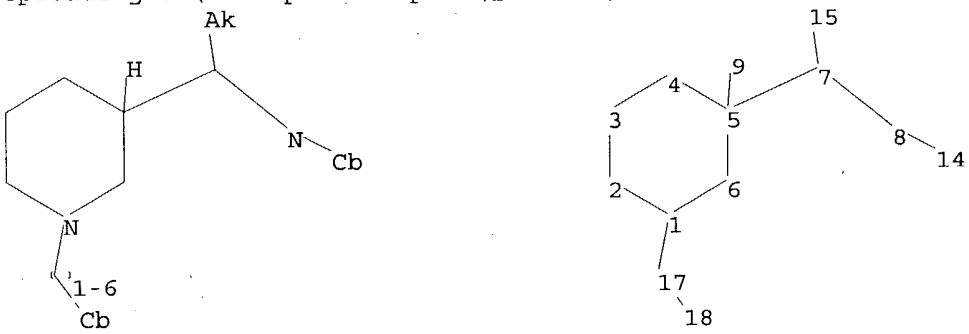
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str



chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18
isolated ring systems :
containing 1 :

G1:H,Ak,Cb

G2:Cb,Ak

G3:H,Ph,Ak

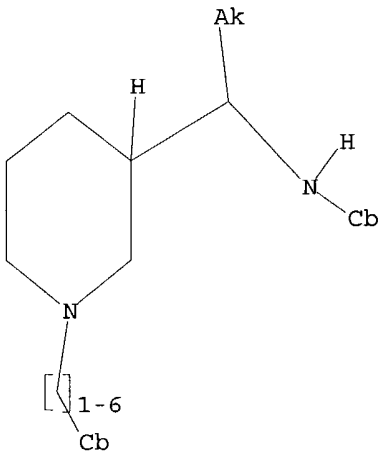
10789414

12/20/04

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS
15:CLASS 17:CLASS 18:Atom

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



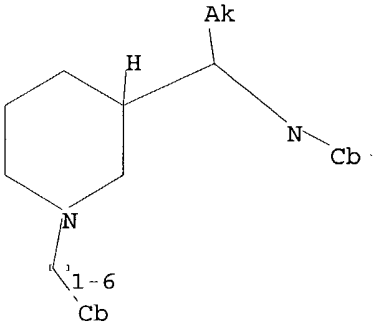
G1 H,Ak,Cb

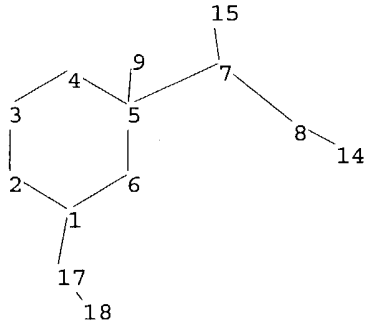
G2 Cb,Ak

G3 H,Ph,Ak

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str





chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :

10789414

12/20/04

1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18
isolated ring systems :
containing 1 :

G1:H,Ak,Cb

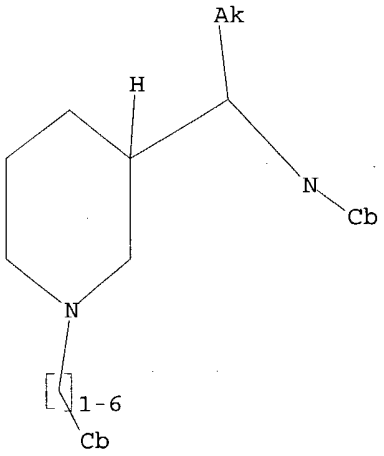
G2:Cb,Ak

G3:H,Ph,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS
15:CLASS 17:CLASS 18:Atom

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G1 H,Ak,Cb

G2 Cb,Ak

G3 H,Ph,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 14:17:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5057 TO ITERATE

10789414

```
 19.8% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        96876 TO   105404
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

=> s l5 ful
FULL SEARCH INITIATED 14:18:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 101916 TO ITERATE

100.0% PROCESSED  101916 ITERATIONS                             11 ANSWERS
SEARCH TIME: 00.00.03

L7           11 SEA SSS FUL L5

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               156.26     312.31

FILE 'CAPLUS' ENTERED AT 14:18:13 ON 20 DEC 2004
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FILE COVERS 1907 - 20 Dec 2004  VOL 141 ISS 26
FILE LAST UPDATED: 19 Dec 2004  (20041219/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l7
L8            5 L7

=> d abs bib hitstr 1-5
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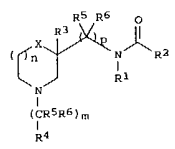
L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
GI



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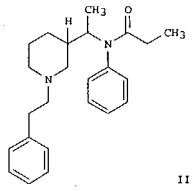
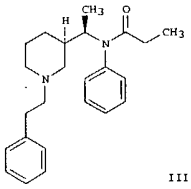


II



III

AB One aspect of the invention relates to novel heterocyclic compds. (6 Markush structures given), e.g., I [wherein: m = 1, 2, 3 or 4; n = 1 or 2; p = 1 or 2; R1 = alkyl, aryl, heteroaryl, or cycloalkyl; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl; R1 and R2 may be connected through a covalent bond; R3 = H, alkyl, aryl, OR2, OC(O)R2CH2OR2, or CO2R2; wherein any 2 instances of R3 may be connected by a covalent tether whose backbone consists of 1, 2, 3, or 4 C atoms; R4 = H, alkyl, aryl, heteroaryl, alkenyl, or cycloalkyl; R5 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; R6 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; Y = OR2, N(R2)2, SR2, S(O)R2, S(O)2R2, or P(O)(OR2)2; a covalent bond may connect R4 and an instance of R5 or R6 that is attached to the C chain between R4 and the ring N explicitly shown; any 2 geminal or vicinal instances of R5 and R6 may be connected through a covalent bond; X = C(R3)2, O, S, SO, SO2, NR2, NC(O)OR2, or C:O; and the stereochem. configuration at any stereocenter is (R)-, (S)-, or mixed]. A second aspect of the invention relates to the use of the compds. as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An addnl. aspect of the invention relates to the use of the compds. as analgesics. A large no. of synthetic and biol. examples are given, including a combinatorial prepn. For instance, 3-(1-hydroxyethyl)piperidine-1-carboxylic acid tert-Bu ester was converted to its mesylate ester, and this reacted with aniline to give 3-[1-(phenylamino)ethyl]piperidine-1-carboxylic acid tert-Bu ester. Amidation of this with propionyl chloride, deprotection of the BOC group with CF3CO2H, and N-alkylation with PhCH2CH2Br, gave the invention compd. II. All 4 enantiomers of II were prepd. by a stereospecific synthesis, and X-ray crystallog. detn. of one enantiomer allowed the abs. stereochem. of its epimer, III, to be assigned. III showed an ED50 of <500 μg/kg (i.v.) in the tail flick assay in rats, which was comparable to fentanyl. The respiratory depression activity (side effect) of 14 invention compds. was also detd. An orally bioavailable formulation of III was studied in rats. A combinatorial library of 96 compds. I was prepd. from 12 anilines and 8 acid chlorides.

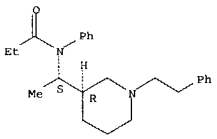
AN 2003:887681 CAPLUS
DN 139:364834
TI Heterocyclic analgesic compounds, namely N-[1-(1-phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide and analogs, with activity at opioid receptors, and method of use thereof
IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjiang; Bannister, Thomas D.
PA Sepracor Inc., USA
SO U.S., 91 pp., Cont.-in-part of U.S. Ser. No. 579,398.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6645980	B1	20031111	US 2000-717174	20001120
	US 6677332	B1	20040113	US 2000-579398	20000525
	US 2002016337	A1	20020207	US 2001-798803	20010302
	US 6635661	B2	20031021		
	US 2003069418	A1	20030410	US 2002-121029	20020411
PRAI	US 2000-579398	A2	20000525		
	US 1999-135721P	P	19990525		
	US 1999-168979P	P	19991203		
	US 2000-195809P	P	20000411		
	US 2000-717174	A2	20001120		
	US 2001-798803	A2	20010302		
	US 2001-284374P	P	20010417		

OS MARPAT 139:364834
IT **309746-87-0P**
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam

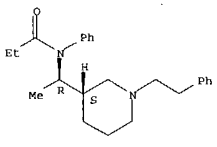
L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
ides and analogs as analgesics)
RN 309746-87-0 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **309746-92-7P**
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-92-7 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

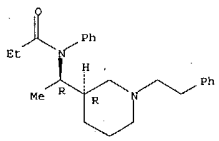
Absolute stereochemistry.



IT **309746-85-8P**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-85-8 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

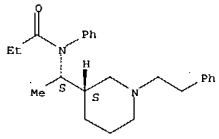
Absolute stereochemistry.

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



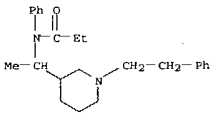
IT **309746-90-5P**
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-90-5 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



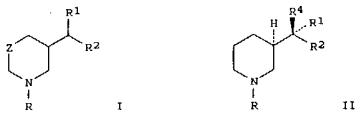
IT **309746-45-0P**, N-[1-(1-Phenethylpiperidine-3-yl)ethyl]-N-phenylpropionamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-45-0 CAPLUS
CN Propanamide, N-phenyl-N-[1-[1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
GI



AB Title compds. [diastereomeric I; R = H, aralkyl, CO2R1; R1 = alkyl or aryl(alkyl); R2 = OH or NHR3; R3 = H, alkyl, aryl(alkyl); Z = bond, CH2, CH2CH2] were prepared Thus, (R)-nipecotic acid Et ester L-tartrate was converted in 3 steps to piperidinecarboxaldehyde II (R = Cbz, R1R4 = O, R2 = H) which was treated with Me2Zn in the presence of (4S)-TADDOL and Ti(OCHMe2)4 to give 62% II (R = Cbz, R1 = Me, R2 = OH, R4 = H) of 90.1% de. The latter was converted to opioid receptor ligand II (R = CH2CH2Ph, R1 = H, R2 = NPhCOEt, R4 = Me). Data for biol. activity of opioid receptor ligands were given.
AN 2002:449649 CAPLUS
DN 137:20299
TI Preparation of α-methylpiperidine-3-methanol diastereomers and analogs as drug intermediates
IN Wu, Xinhe; Bannister, Thomas D.; Cuny, Gregory D.; Shao, Liming; Aquila, Brian M.; Hauske, James R.; Hefferman, Michele L.; Xie, Roger L.; Kessler, Donald W.; Hoemann, Michael Z.
PA Sepracor, Inc., USA
SO PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002046157	A2	20020613	WO 2001-US47037	20011204
	WO 2002046157	A3	20030227		
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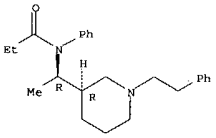
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002037704	A5	20020618	AU 2002-37704	20011204
	US 2002177721	A1	20021128	US 2001-12242	20011204
	US 6703508	B2	20040309		
	US 2004235893	A1	20041125	US 2004-789414	20040227

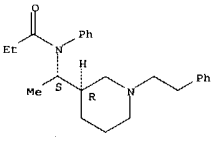
L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
PRAI US 2000-251209P P 20001204
US 2001-275600P P 20010313
US 2001-12242 A3 20011204
WO 2001-US47037 W 20011204
OS CASREACT 137:20299; MARPAT 137:20299
IT **309746-85-8P 309746-87-0P 309746-90-5P**
309746-92-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of α-methylpiperidine-3-methanol diastereomers and analogs as drug intermediates)
RN 309746-85-8 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 309746-87-0 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

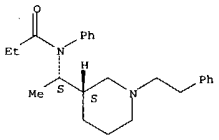
Absolute stereochemistry.



RN 309746-90-5 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

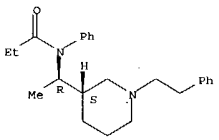
Absolute stereochemistry.

L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

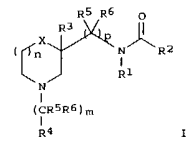


RN 309746-92-7 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
GI



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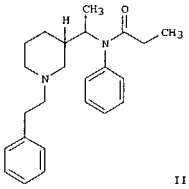

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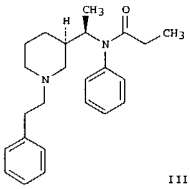

III

AB One aspect of the invention relates to novel heterocyclic compds. (6 Markush structures given), e.g., I [wherein: m = 1, 2, 3 or 4; n = 1 or 2;
p = 1 or 2; R1 = alkyl, aryl, heteroaryl, or cycloalkyl; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl; R1 and R2 may be connected through a covalent bond; R3 = H, alkyl, aryl, OR2, OC(O)R2CH2OR2, or CO2R2; wherein any 2 instances of R3 may be connected by a covalent tether
whose backbone consists of 1, 2, 3, or 4 C atoms; R4 = H, alkyl, aryl, heteroaryl, alkenyl, or cycloalkyl; R5 = H, alkyl, CH2Y, aryl, heteroaryl,
F, OR2, or OC(O)R2; R6 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; Y = OR2, N(R2)2, SR2, S(O)R2, S(O)2R2, or P(O)(OR2)2; a covalent bond may connect R4 and an instance of R5 or R6 that is attached to the C chain between R4 and the ring N explicitly shown; any 2 geminal or vicinal
instances of R5 and R6 may be connected through a covalent bond; X = C(R3)2, O, S, SO, SO2, NR2, NC(O)OR2, or C:O; and the stereochem. configuration at any stereocenter is (R)-, (S)-, or mixed]. A second aspect of the invention relates to the use of the compds. as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An addnl. aspect of the invention relates to the use of the compds. as analgesics. A large no. of
synthetic and biol. examples are given, including a combinatorial prepn. For instance, 3-(1-hydroxyethyl)piperidine-1-carboxylic acid tert-Bu ester
was converted to its mesylate ester, and this reacted with aniline to give
3-[1-(phenylamino)ethyl]piperidine-1-carboxylic acid tert-Bu ester. Amidation of this with propionyl chloride, deprotection of the BOC group with CF3CO2H, and N-alkylation with PhCH2CH2Br, gave the invention compd. II. All 4 enantiomers of II were prepd. by a stereospecific synthesis, and X-ray crystallog. detn. of one enantiomer allowed the abs. stereochem.
of its epimer, III, to be assigned. III showed an ED50 of <500 μg/kg (i.v.) in the tail flick assay in rats, which was comparable to fentanyl. The respiratory depression activity (side effect) of 14 invention compds. was also detd. An orally bioavailable formulation of III was studied in rats. A combinatorial library of 96 compds. I was prepd. from 12 anilines
and 8 acid chlorides.

AN 2002:107910 CAPLUS
DN 136:167282
TI Heterocyclic analgesic compounds, namely N-[1-(1-phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide and analogs, with activity as opioid receptors, and method of use thereof
IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjiang; Bannister, Thomas D.
PA Sepracor, Inc., USA
SO U.S. Pat. Appl. Publ., 107 pp., Cont.-in-part of U.S. Ser. No. 717,174.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002016337	A1	20020207	US 2001-798803	20010302
	US 6635661	B2	20031021		
	US 6677332	B1	20040113	US 2000-579398	20000525
	US 6645980	B1	20031111	US 2000-717174	20001120
	WO 2002069895	A2	20020912	WO 2002-US6274	20020301
	WO 2002069895	A3	20021031		
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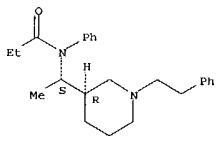
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003069418	A1	20030410	US 2002-121029	20020411
PRAI	US 2000-579398	A2	20000525		
	US 2000-717174	A2	20001120		
	US 1999-135721P	P	19990525		

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

	US 1999-168979P	P	19991203
	US 2000-195809P	P	20000411
	US 2001-798803	A	20010302
	US 2001-284374P	P	20010417

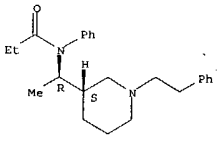
OS MARPAT 136:167282
IT **309746-87-0P**, Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]-
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-87-0 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **309746-92-7P**, Propanamide, N-phenyl-N-[(1R)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]-
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-92-7 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

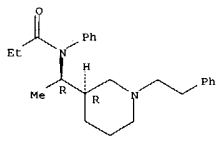
Absolute stereochemistry.



L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

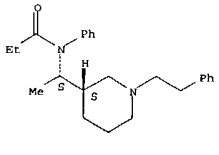
IT **309746-85-8P**, Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]-
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-85-8 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



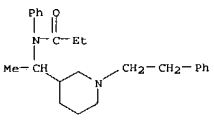
IT **309746-90-5P**, Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]-
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-90-5 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



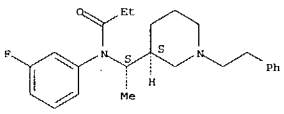
IT **309746-45-0P**, N-[1-(1-Phenethylpiperidine-3-yl)ethyl]-N-phenylpropionamide **395682-22-1P 395682-23-2P 395682-24-3P 395682-25-4P 395682-26-5P 395682-27-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(drug candidate; prepn. of [(phenethylpiperidinyl)ethyl]phenylpropionamides and analogs as analgesics)
RN 309746-45-0 CAPLUS
CN Propanamide, N-phenyl-N-[1-[1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)



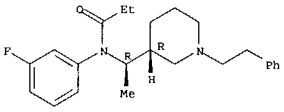
RN 395682-22-1 CAPLUS
CN Propanamide, N-(3-fluorophenyl)-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 395682-23-2 CAPLUS
CN Propanamide, N-(3-fluorophenyl)-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

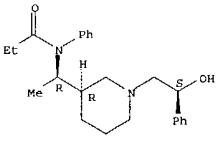
Absolute stereochemistry.



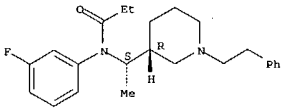
RN 395682-24-3 CAPLUS
CN Propanamide, N-(3-fluorophenyl)-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 395682-25-4 CAPLUS
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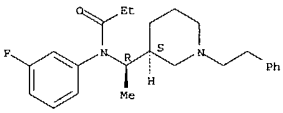
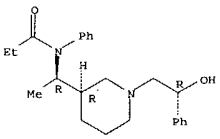
Absolute stereochemistry.



RN 395682-26-5 CAPLUS
CN Propanamide, N-[(1R)-1-[(3R)-1-[(2R)-2-hydroxy-2-phenylethyl]-3-piperidinyl]ethyl]-N-phenyl- (9CI) (CA INDEX NAME)

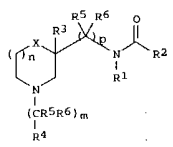
Absolute stereochemistry.



RN 395682-27-6 CAPLUS
CN Propanamide, N-[(1R)-1-[(3R)-1-[(2S)-2-hydroxy-2-phenylethyl]-3-piperidinyl]ethyl]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
GI



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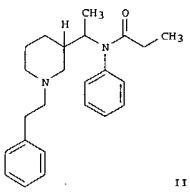
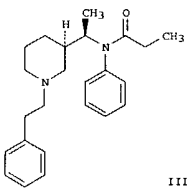


II



III

AB One aspect of the invention relates to novel heterocyclic compds. (6 Markush structures given), e.g., I [wherein: m = 1, 2, 3 or 4; n = 1 or 2; p = 1 or 2; R1 = alkyl, aryl, heteroaryl, or cycloalkyl; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl; R1 and R2 may be connected through a covalent bond; R3 = H, alkyl, aryl, OR2, OC(O)R2CH2OR2, or CO2R2; wherein any 2 instances of R3 may be connected by a covalent tether whose backbone consists of 1, 2, 3, or 4 C atoms; R4 = H, alkyl, aryl, heteroaryl, alkenyl, or cycloalkyl; R5 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; R6 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; Y = OR2, N(R2)2, SR2, S(O)R2, S(O)2R2, or P(O)(OR2)2; a covalent bond may connect R4 and an instance of R5 or R6 that is attached to the C chain between R4 and the ring N explicitly shown; any 2 geminal or vicinal instances of R5 and R6 may be connected through a covalent bond; X = C(R3)2, O, S, SO, SO2, NR2, NC(O)OR2, or C:O; and the stereochem. configuration at any stereocenter is (R)-, (S)-, or mixed]. A second aspect of the invention relates to the use of the compds. as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An addnl. aspect of the invention relates to the use of the compds. as analgesics. A large number of synthetic and biol. examples are given, including a combinatorial preparation

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
For instance, 3-(1-hydroxyethyl)piperidine-1-carboxylic acid tert-Bu ester
was converted to its mesylate ester, and this reacted with aniline to give
3-[1-(phenylamino)ethyl]piperidine-1-carboxylic acid tert-Bu ester. Amidation of this with propionyl chloride, deprotection of the BOC group with CF3CO2H, and N-alkylation with PhCH2CH2Br, gave the invention compd. II. All 4 enantiomers of II were prepd. by a stereospecific synthesis, and X-ray crystallog. detn. of one enantiomer allowed the abs. stereochem.
of its epimer, III, to be assigned. III showed an ED50 of <500 μg/kg (i.v.) in the tail flick assay in rats, which was comparable to fentanyl. The respiratory depression activity (side effect) of 14 invention compds. was also detd. An orally bioavailable formulation of III was studied in rats. A combinatorial library of 96 compds. I was prepd. from 12 anilines
and 8 acid chlorides.
AN 2001:886067 CAPLUS
DN 136:20020
TI Heterocyclic analgesic compounds, namely N-[1-(1-phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide and analogs, with activity at opioid receptors, and method of use thereof
IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjian; Bannister, Thomas D.
PA Sepracor, Inc., USA
SO PCT Int. Appl., 229 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 6

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001092226	A1	20011206	WO 2000-US31724	20001120
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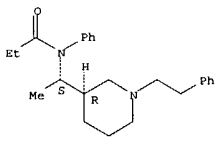
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6677332	B1	20040113	US 2000-579198	20000525
PRAI US 2000-579398	A	20000525		
US 1999-135721P	P	19990525		
US 1999-168979P	P	19991203		
US 2000-195809P	P	20000411		

OS MARPAT 136:20020
IT **309746-87-0P**
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam

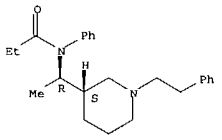
L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
ides and analogs as analgesics)
RN 309746-87-0 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **309746-92-7P**
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation), USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-92-7 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

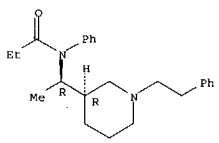
Absolute stereochemistry.



IT **309746-85-8P**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-85-8 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

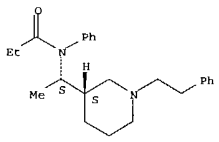
L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Absolute stereochemistry.



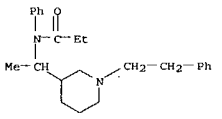
IT **309746-90-5P**
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-90-5 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **309746-45-0P**, N-[1-(1-Phenethylpiperidine-3-yl)ethyl]-N-phenylpropionamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionam
ides and analogs as analgesics)
RN 309746-45-0 CAPLUS
CN Propanamide, N-phenyl-N-[1-[1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention discloses novel nitrogen heterocycles of formula I (A = (CH2)b, Z = (CH2)y, W = (CH2)n, where b = 0 or 1, yr = 1 or 2, and n = 1, 2 or 3 with provisions; X = C(R3)2, O, S, SO2, NR2, NCO2R2, or CO; R1
= alkyl, aryl, heteroaryl, or cycloalkyl; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl; R1 and R2 may be connected via covalent bond; R3 = H, alkyl, aryl, OR2, OCOR2, CH2OR2, or CO2R2, wherein any two instances of R3 may be connected via divalent carbon bridge; R4 = H, alkyl, aryl, heteroaryl, alkenyl, or cycloalkyl; R5 or R6 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2 or OCOR2; Y = OR2, N(R2)2, SR2, SOR2, SO2R2
or PO(OR2)2; R4 may be covalently attached to an adjacent R5 or R6; p = 1,
2, 3 or 4; m = 0, 1, or 2) and II (y = 1; n = 2; b = 0) as well as methods
for preparation Compound III was prepared by successive amidation of (R)-N-(1-Boc-piperidin-3-ylmethyl)aniline, deprotection and alkylation. Methods employed to prepare claimed compds. included combinatorial chemical
providing ninety-six piperidinyl deriva. with IC50 values (μM) ranging 0.31-5.76 and 0.08-4 against κ and μ opioid receptors, resp. III was five times stronger [ED50 (μg/kg) <500] than morphine [ED50 <2500] as an analgesic as demonstrated in a standard rat tail flick test. A second
aspect of the present invention relates to the use of the novel heterocyclic compds. as ligands for various cellular receptors, including opiate receptors, other the G-protein coupled receptors, and ion channels.
An addnl. aspect of the invention relates to the use of the novel heterocyclic compds. as analgesics.

AN 2000:842113 CAPLUS
DN 134:29315
TI Heterocyclic analgesic compounds and methods of use thereof
IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjian; Bannister, Thomas D.
PA Sepracor, Inc., USA
SO PCT Int. Appl., 216 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000071518	A2	20001130	WO 2000-US14579	20000525
	WO 2000071518	A3	20011018		

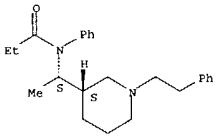
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

	CA 2372887	AA	20001130	CA 2000-2372887	20000525
	EP 1187810	A2	20020320	EP 2000-937830	20000525
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2003500392	T2	20030107	JP 2000-619775	20000525
PRAI	US 1999-135721P	P	19990525		
	US 1999-168979P	P	19991203		
	US 2000-195809P	P	20000411		
	WO 2000-US14579	W	20000525		

OS MARPAT 134:29315
IT **309746-90-5P 309746-92-7P**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and biol. activity of nitrogen heterocyclic analgesic compds.)
RN 309746-90-5 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

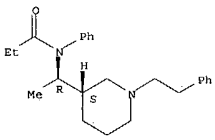
Absolute stereochemistry.



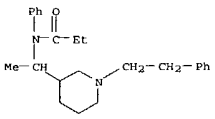
RN 309746-92-7 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

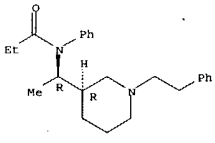


IT **309746-45-0P 309746-85-8P 309746-87-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and biol. activity of nitrogen heterocyclic analgesic compds.)
RN 309746-45-0 CAPLUS
CN Propanamide, N-phenyl-N-[1-[1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)



RN 309746-85-8 CAPLUS
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

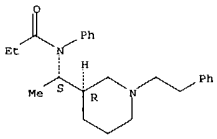
Absolute stereochemistry.



RN 309746-87-0 CAPLUS
CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



12/20/04

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=> file uspatall
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                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      25.12     337.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                      -3.50      -3.50

FILE 'USPATFULL' ENTERED AT 14:20:07 ON 20 DEC 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 14:20:07 ON 20 DEC 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d his

     (FILE 'HOME' ENTERED AT 14:14:56 ON 20 DEC 2004)

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L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FUL

     FILE 'REGISTRY' ENTERED AT 14:16:26 ON 20 DEC 2004
L4             STRUCTURE UPLOADED
L5             STRUCTURE UPLOADED
L6           0 S L5
L7          11 S L5 FUL

     FILE 'CAPLUS' ENTERED AT 14:18:13 ON 20 DEC 2004
L8           5 S L7

     FILE 'USPATFULL, USPAT2' ENTERED AT 14:20:07 ON 20 DEC 2004

=> s l7
L9           8 L7

=> d abs bib fhitstr 1-8
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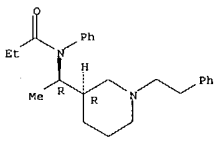
L9 ANSWER 1 OF 8 USPATFULL on STN

AB One aspect of the present invention relates to methods of synthesizing substituted piperidines. A second aspect of the present invention relates to stereoselective methods of synthesizing substituted piperidines. The methods of the present invention will find use in the synthesis of compounds useful for treatment of numerous ailments, conditions and diseases that afflict mammals, including but not limited to addiction and pain. An additional aspect of the present invention relates to the synthesis of combinatorial libraries of the substituted piperidines using the methods of the present invention. An additional aspect of the present invention relates to enantiomerically substituted pyrrolidines, piperidines, and azepines.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AN 2004:300024 USPATFULL
TI Methods for the stereoselective synthesis of substituted piperidines
IN Aquila, Brian M., Marlborough, MA, UNITED STATES
Bannister, Thomas D., Northborough, MA, UNITED STATES
Cuny, Gregory D., Somerville, MA, UNITED STATES
Hauske, James R., Concord, MA, UNITED STATES
Heffernan, Michele L.R., Worcester, MA, UNITED STATES
Hoemann, Michael Z., Marlborough, MA, UNITED STATES
Kessler, Donald W., Groton, MA, UNITED STATES
Shao, Liming, Lincoln, MA, UNITED STATES
Wu, Xinhe, Shrewsbury, MA, UNITED STATES
Xie, Roger L., Natick, MA, UNITED STATES
PI US 2004235893 A1 20041125
AI US 2004-789414 A1 20040227 (10)
RLI Division of Ser. No. US 2001-12242, filed on 4 Dec 2001, GRANTED, Pat. No. US 6703508
PRAI US 2000-251209P 20001204 (60)
US 2001-275600P 20010313 (60)
DT Utility
FS APPLICATION
LREP FOLEY HOAG, LLP, PATENT GROUP, WORLD TRADE CENTER WEST, 155 SEAPORT BLVD, BOSTON, MA, 02110
CLMN Number of Claims: 104
ECL Exemplary Claim: 1
DRWN 41 Drawing Page(s)
LN.CNT 2533
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **309746-85-8P**
(preparation of α-methylpiperidine-3-methanol diastereomers and analogs as drug intermediates)
RN 309746-85-8 USPATFULL
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 1 OF 8 USPATFULL on STN (Continued)

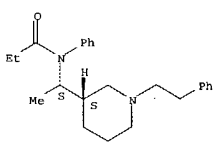


L9 ANSWER 2 OF 8 USPATFULL on STN

AB One aspect of the present invention relates to novel heterocyclic compounds. A second aspect of the present invention relates to the use of the novel heterocyclic compounds as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An additional aspect of the present invention relates to the use of the novel heterocyclic compounds as analgesics.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AN 2004:268303 USPATFULL
TI Heterocyclic analgesic compounds and methods of use thereof
IN Cuny, Gregory D., Hudson, MA, UNITED STATES
Shao, Liming, Lincoln, MA, UNITED STATES
Hauske, James R., Concord, MA, UNITED STATES
Heffernan, Michele L.R., Framingham, MA, UNITED STATES
Aquila, Brian M., Marlborough, MA, UNITED STATES
Wu, Xinhe, Shrewsbury, MA, UNITED STATES
Wang, Fengjiang, Northborough, MA, UNITED STATES
Bannister, Thomas D., Northborough, MA, UNITED STATES
PI US 2004209846 A1 20041021
AI US 2004-754101 A1 20040107 (10)
RLI Division of Ser. No. US 2000-579398, filed on 25 May 2000, GRANTED, Pat.
No. US 6677332
PRAI US 2000-195809P 20000411 (60)
US 1999-168979P 19991203 (60)
US 1999-135721P 19990525 (60)
DT Utility
FS APPLICATION
LREP FOLEY HOAG, LLP, PATENT GROUP, WORLD TRADE CENTER WEST, 155 SEAPORT BLVD, BOSTON, MA, 02110
CLMN Number of Claims: 204
ECL Exemplary Claim: 1
DRWN 3 Drawing Page(s)
LN.CNT 6866
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **309746-90-5P**
(preparation and biol. activity of nitrogen heterocyclic analgesic compds.)
RN 309746-90-5 USPATFULL
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

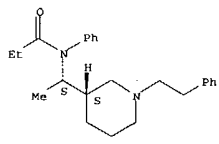


L9 ANSWER 3 OF 8 USPATFULL on STN

AB One aspect of the present invention relates to novel heterocyclic compounds. A second aspect of the present invention relates to the use of the novel heterocyclic compounds as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An additional aspect of the present invention relates to the use of the novel heterocyclic compounds as analgesics.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AN 2004:9609 USPATFULL
TI Heterocyclic analgesic compounds and methods of use thereof
IN Cuny, Gregory D., Hudson, MA, United States
Shao, Liming, Lincoln, MA, United States
Hauske, James R., Concord, MA, United States
Heffernan, Michele L. R., Framingham, MA, United States
Aquila, Brian M., Marlborough, MA, United States
Wu, Xinhe, Marlborough, MA, United States
Wang, Fengjiang, Northborough, MA, United States
Bannister, Thomas D., Northborough, MA, United States
PA Sepracor, Inc., Marlborough, MA, United States (U.S. corporation)
PI US 6677332 B1 20040113
AI US 2000-579398 20000525 (9)
PRAI US 2000-195809P 20000411 (60)
US 1999-168979P 19991203 (60)
US 1999-135721P 19990525 (60)
DT Utility
FS GRANTED
EXNAM Primary Examiner: Shah, Mukund J.; Assistant Examiner: Liu, Hong
LREP Foley Hoag LLP, Gordon, Dana M.
CLMN Number of Claims: 32
ECL Exemplary Claim: 1
DRWN 3 Drawing Figure(s); 3 Drawing Page(s)
LN.CNT 6122
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **309746-90-5P**
(preparation and biol. activity of nitrogen heterocyclic analgesic compds.)
RN 309746-90-5 USPATFULL
CN Propanamide, N-phenyl-N-[(1S)-1-[(3S)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 8 USPATFULL on STN

AB One aspect of the present invention relates to novel heterocyclic compounds. A second aspect of the present invention relates to the use of the novel heterocyclic compounds as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An additional aspect of the present invention relates to the use of the novel heterocyclic compounds as analgesics.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AN 2003:296935 USPATFULL

TI Heterocyclic analgesic compounds and methods of use thereof

IN Cuny, Gregory D., Hudson, MA, United States
Shao, Liming, Lincoln, MA, United States
Hauske, James R., Concord, MA, United States
Heffernan, Michele L. R., Framingham, MA, United States
Aquila, Brian M., Marlborough, MA, United States
Wu, Xinhe, Shrewsbury, MA, United States
Wang, Fengjiang, Northborough, MA, United States
Bannister, Thomas D., Northborough, MA, United States

PA Sepracor Inc., Marlborough, MA, United States (U.S. corporation)

PI US 6645980 B1 20031111

AI US 2000-717174 20001120 (9)

RLI Continuation-in-part of Ser. No. US 2000-579398, filed on 25 May 2000

DT Utility

FS GRANTED

EXNAM Primary Examiner: Coleman, Brenda

LREP Gordon, Dana M., Foley Hoag LLP

CLMN Number of Claims: 21

ECL Exemplary Claim: 1

DRWN 4 Drawing Figure(s); 4 Drawing Page(s)

LN.CNT 6228

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

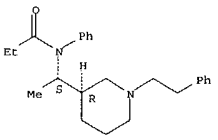
IT **309746-87-0P**

(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionamides and analogs as analgesics)

RN 309746-87-0 USPATFULL

CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 8 USPATFULL on STN (Continued)

L9 ANSWER 5 OF 8 USPATFULL on STN

AB One aspect of the present invention relates to methods of synthesizing substituted piperidines. A second aspect of the present invention relates to stereoselective methods of synthesizing substituted piperidines. The methods of the present invention will find use in the synthesis of compounds useful for treatment of numerous ailments, conditions and diseases that afflict mammals, including but not limited to addiction and pain. An additional aspect of the present invention relates to the synthesis of combinatorial libraries of the substituted piperidines using the methods of the present invention. An additional aspect of the present invention relates to enantiomerically substituted pyrrolidines, piperidines, and azepines.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AN 2002:315232 USPATFULL

TI Methods for the stereoselective synthesis of substituted piperidines

IN Aquila, Brian M., Marlborough, MA, UNITED STATES
Bannister, Thomas D., Northborough, MA, UNITED STATES
Cuny, Gregory C., Somerville, MA, UNITED STATES
Hauske, James R., Concord, MA, UNITED STATES
Heffernan, Michele L.R., Worcester, MA, UNITED STATES
Hoemann, Michael Z., Marlborough, MA, UNITED STATES
Kessler, Donald W., Groton, MA, UNITED STATES
Shao, Liming, Lincoln, MA, UNITED STATES
Wu, Xinhe, Shrewsbury, MA, UNITED STATES
Xie, Roger L., Natick, MA, UNITED STATES

PI US 2002177721 A1 20021128
US 6703508 B2 20040309

AI US 2001-12242 A1 20011204 (10)

PRAI US 2000-251209P 20001204 (60)
US 2001-275600P 20010313 (60)

DT Utility

FS APPLICATION

LREP FOLEY, HOAG & ELIOT, LLP, PATENT GROUP, ONE POST OFFICE SQUARE, BOSTON, MA, 02109

CLMN Number of Claims: 104

ECL Exemplary Claim: 1

DRWN 41 Drawing Page(s)

LN.CNT 2542

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

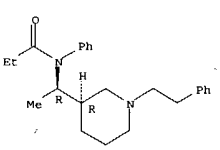
IT **309746-85-8P**

(preparation of α-methylpiperidine-3-methanol diastereomers and analogs as drug intermediates)

RN 309746-85-8 USPATFULL

CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 5 OF 8 USPATFULL on STN (Continued)

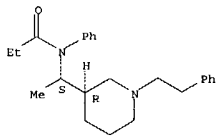
L9 ANSWER 6 OF 8 USPATFULL on STN

AB One aspect of the present invention relates to novel heterocyclic compounds. A second aspect of the present invention relates to the use of the novel heterocyclic compounds as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An additional aspect of the present invention relates to the use of the novel heterocyclic compounds as analgesics.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AN 2002:27489 USPATFULL
TI Heterocyclic analgesic compounds and methods of use thereof
IN Cuny, Gregory D., Hudson, MA, UNITED STATES
Shao, Liming, Lincoln, MA, UNITED STATES
Hauske, James R., Concord, MA, UNITED STATES
Heffernan, Michele L.R., Worcester, MA, UNITED STATES
Aquila, Brian M., Marlborough, MA, UNITED STATES
Wu, Xinhe, Shrewsbury, MA, UNITED STATES
Wang, Fengjiang, Northborough, MA, UNITED STATES
Bannister, Thomas D., Northborough, MA, UNITED STATES
PI US 2002016337 A1 20020207
US 6635661 B2 20031021
AI US 2001-798803 A1 20010302 (9)
RLI Continuation-in-part of Ser. No. US 2000-717174, filed on 20 Nov 2000, PENDING Continuation-in-part of Ser. No. US 2000-579398, filed on 25 May
2000, PENDING
DT Utility
FS APPLICATION
LREP FOLEY, HOAG & ELIOT, LLP, PATENT GROUP, ONE POST OFFICE SQUARE, BOSTON, MA, 02109
CLMN Number of Claims: 26
ECL Exemplary Claim: 1
DRWN 4 Drawing Page(s)
LN.CNT 6366
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **309746-87-0P**, Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]-
(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionamides and analogs as analgesics)
RN 309746-87-0 USPATFULL
CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 6 OF 8 USPATFULL on STN (Continued)



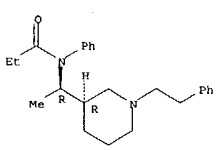
L9 ANSWER 7 OF 8 USPAT2 on STN

AB One aspect of the present invention relates to methods of synthesizing substituted piperidines. A second aspect of the present invention relates to stereoselective methods of synthesizing substituted piperidines. The methods of the present invention will find use in the synthesis of compounds useful for treatment of numerous ailments, conditions and diseases that afflict mammals, including but not limited to addiction and pain. An additional aspect of the present invention relates to the synthesis of combinatorial libraries of the substituted piperidines using the methods of the present invention. An additional aspect of the present invention relates to enantiomerically substituted pyrrolidines, piperidines, and azepines.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AN 2002:315232 USPAT2
TI Methods for the stereoselective synthesis of substituted piperidines
IN Aquila, Brian M., Marlborough, MA, United States
Bannister, Thomas D., Northborough, MA, United States
Cuny, Gregory D., Somerville, MA, United States
Hauske, James R., Concord, MA, United States
Heffernan, Michelle L. R., Worcester, MA, United States
Hoemann, Michael Z., Marlborough, MA, United States
Kessler, Donald W., Groton, MA, United States
Shao, Liming, Lincoln, MA, United States
Wu, Xinhe, Shrewsbury, MA, United States
Xie, Roger L., Natick, MA, United States
PA Sepracor, Inc., Marlborough, MA, United States (U.S. corporation)
PI US 6703508 B2 20040309
AI US 2001-12242 20011204 (10)
PRAI US 2000-251209P 20001204 (60)
US 2001-275600P 20010313 (60)
DT Utility
FS GRANTED
EXNAM Primary Examiner: Desai, Rita
LREP Gordon, Dana M., Foley Hoag LLP
CLMN Number of Claims: 32
ECL Exemplary Claim: 1
DRWN 41 Drawing Figure(s); 41 Drawing Page(s)
LN.CNT 2363
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **309746-85-8P**
(preparation of α-methylpiperidine-3-methanol diastereomers and analogs as drug intermediates)
RN 309746-85-8 USPAT2
CN Propanamide, N-phenyl-N-[(1R)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L9 ANSWER 7 OF 8 USPAT2 on STN (Continued)



L9 ANSWER 8 OF 8 USPAT2 on STN

AB One aspect of the present invention relates to novel heterocyclic compounds. A second aspect of the present invention relates to the use of the novel heterocyclic compounds as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An additional aspect of the present invention relates to the use of the novel heterocyclic compounds as analgesics.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AN 2002:27489 USPAT2

TI Heterocyclic analgesic compounds and methods of use thereof

IN Cuny, Gregory D., Hudson, MA, United States
Shao, Liming, Lincoln, MA, United States
Hauske, James R., Concord, MA, United States
Heffernan, Michele L. R., Worcester, MA, United States
Aquila, Brian M., Marlborough, MA, United States
Wu, Xinhe, Shrewsbury, MA, United States
Wang, Fengjiang, Northborough, MA, United States
Bannister, Thomas D., Northborough, MA, United States

PA Sepracor Inc., Marlborough, MA, United States (U.S. corporation)

PI US 6635661 B2 20031021

AI US 2001-798803 20010302 (9)

RLI Continuation-in-part of Ser. No. US 2000-717174, filed on 20 Nov 2000
Continuation-in-part of Ser. No. US 2000-579398, filed on 25 May 2000

DT Utility

FS GRANTED

EXNAM Primary Examiner: Coleman, Brenda

LREP Gordon, Dana M., Foley Hoag LLP

CLMN Number of Claims: 26

ECL Exemplary Claim: 1

DRWN 4 Drawing Figure(s); 4 Drawing Page(s)

LN.CNT 6279

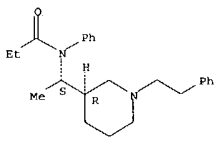
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **309746-87-0P**, Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionamides and analogs as analgesics)

RN 309746-87-0 USPAT2

CN Propanamide, N-phenyl-N-[(1S)-1-[(3R)-1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 8 OF 8 USPAT2 on STN (Continued)

12/20/04

=> logoff y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.86	383.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.50

STN INTERNATIONAL LOGOFF AT 14:20:42 ON 20 DEC 2004

12/20/04

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612rxd

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  SEP 01   New pricing for the Save Answers for SciFinder Wizard within
                   STN Express with Discover!
 NEWS  4  OCT 28   KOREAPAT now available on STN
 NEWS  5  NOV 18   Current-awareness alerts, saved answer sets, and current
                   search transcripts to be affected by CERAB, COMPUAB, ELCOM,
                   and SOLIDSTATE reloads
 NEWS  6  NOV 30   PHAR reloaded with additional data
 NEWS  7  DEC 01   LISA now available on STN
 NEWS  8  DEC 09   12 databases to be removed from STN on December 31, 2004
 NEWS  9  DEC 15   MEDLINE update schedule for December 2004
 NEWS  10 DEC 17   ELCOM reloaded; updating to resume; current-awareness
                   alerts (SDIs) affected
 NEWS  11 DEC 17   COMPUAB reloaded; updating to resume; current-awareness
                   alerts (SDIs) affected
 NEWS  12 DEC 17   SOLIDSTATE reloaded; updating to resume; current-awareness
                   alerts (SDIs) affected
 NEWS  13 DEC 17   CERAB reloaded; updating to resume; current-awareness
                   alerts (SDIs) affected
 NEWS  14 DEC 17   THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB

 NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:28:05 ON 20 DEC 2004
```

10789414

12/20/04

=> file registry
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 0.21 | 0.21

FILE 'REGISTRY' ENTERED AT 12:28:14 ON 20 DEC 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

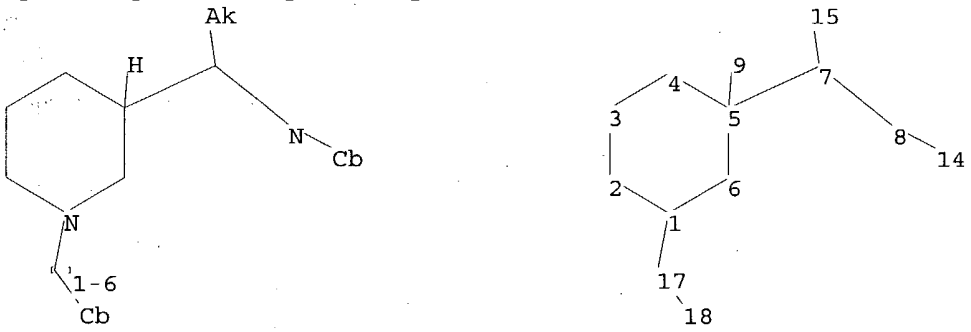
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str



chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18
isolated ring systems :
containing 1 :

G1:H,Ak,Cb

10789414

12/20/04

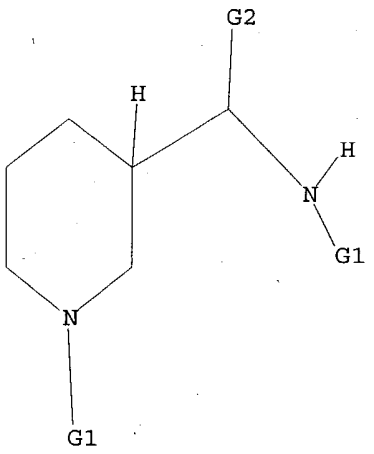
G2:Cb,Ak

G3:H,Ph,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS
15:CLASS 17:CLASS 18:Atom

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Ak,Cb

G2 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 12:28:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 20126 TO ITERATE

5.0% PROCESSED 1000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 394031 TO 411009
PROJECTED ANSWERS: 425 TO 1185

L2 2 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 12:28:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 402724 TO ITERATE

12/20/04

```
 99.3% PROCESSED  400000 ITERATIONS                          143 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.07

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       402724 TO   402724
PROJECTED ANSWERS:             143 TO      178

L3          143 SEA SSS FUL L1

=>
Connection closed by remote host

Connecting via Winsock to STN



Welcome to STN International!  Enter x:x

LOGINID:ssspta1612rxd

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2          "Ask CAS" for self-help around the clock
 NEWS  3  SEP 01  New pricing for the Save Answers for SciFinder Wizard within
                  STN Express with Discover!
 NEWS  4  OCT 28  KOREAPAT now available on STN
 NEWS  5  NOV 18  Current-awareness alerts, saved answer sets, and current
                  search transcripts to be affected by CERAB, COMPUAB, ELCOM,
                  and SOLIDSTATE reloads
 NEWS  6  NOV 30  PHAR reloaded with additional data
 NEWS  7  DEC 01  LISA now available on STN
 NEWS  8  DEC 09  12 databases to be removed from STN on December 31, 2004
 NEWS  9  DEC 15  MEDLINE update schedule for December 2004
 NEWS  10 DEC 17  ELCOM reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  11 DEC 17  COMPUAB reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  12 DEC 17  SOLIDSTATE reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  13 DEC 17  CERAB reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  14 DEC 17  THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB

 NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)
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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:24:35 ON 20 DEC 2004

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	0.84

FILE 'REGISTRY' ENTERED AT 13:27:09 ON 20 DEC 2004
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STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.94	3.78

FILE 'REGISTRY' ENTERED AT 13:31:10 ON 20 DEC 2004
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STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

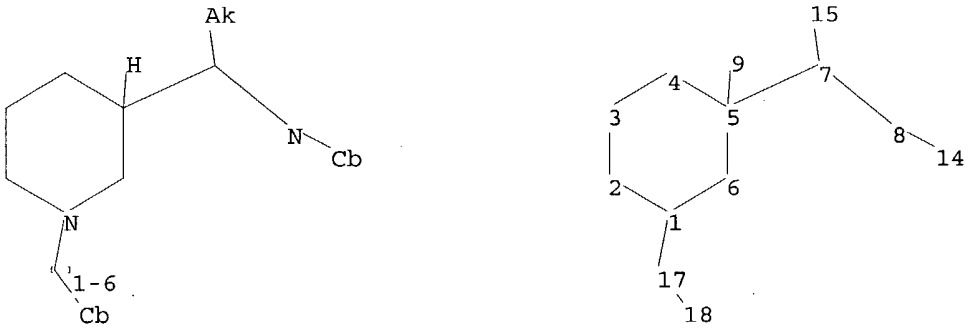
12/20/04

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str



chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18
isolated ring systems :
containing 1 :

G1:H,Ak,Cb

G2:Cb,Ak

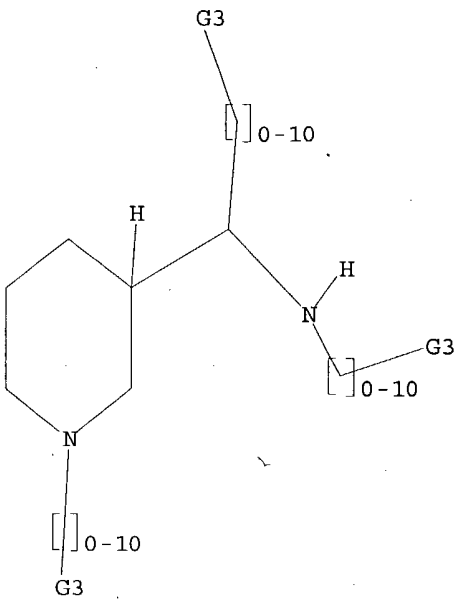
G3:H,Ph,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS
15:CLASS 17:CLASS 18:Atom

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

10789414



G1 H,Ak,Cb

G2 Cb,Ak

G3 H,Ph

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 13:31:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 194218 TO ITERATE

  0.5% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L2             0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 13:31:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

<   9.7% PROCESSED  375033 ITERATIONS                             164 ANSWERS

<  10.3% PROCESSED  400000 ITERATIONS                             173 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.18

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
```

12/20/04

PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 1557

L3 173 SEA SSS FUL L1

=> file registry
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	157.52	161.30

FILE 'REGISTRY' ENTERED AT 13:34:36 ON 20 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

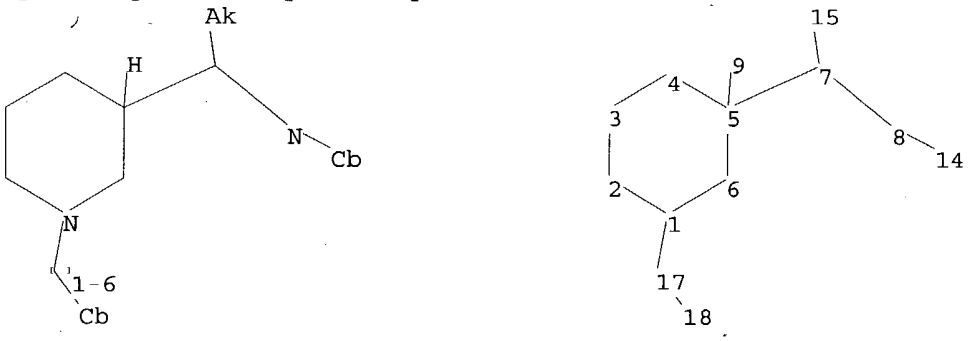
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str



chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18

10789414

12/20/04

isolated ring systems :
containing 1 :

G1:H,Ak,Cb

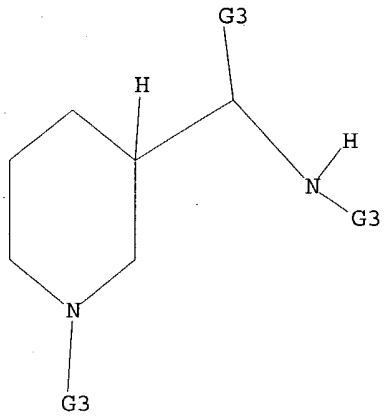
G2:Cb,Ak

G3:H,Ph,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS
15:CLASS 17:CLASS 18:Atom

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



G1 H,Ak,Cb

G2 Cb,Ak

G3 H,Ph,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 13:34:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 20126 TO ITERATE

5.0% PROCESSED 1000 ITERATIONS 8 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 394031 TO 411009
PROJECTED ANSWERS: 2459 TO 3981

12/20/04

L5 8 SEA SSS SAM L4

=> s l4 ful
FULL SEARCH INITIATED 13:34:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 402724 TO ITERATE

99.3% PROCESSED 400000 ITERATIONS 2320 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.08

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 402724 TO 402724
PROJECTED ANSWERS: 2320 TO 2479

L6 2320 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 155.42 316.72

FILE 'CAPLUS' ENTERED AT 13:35:10 ON 20 DEC 2004
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FILE COVERS 1907 - 20 Dec 2004 VOL 141 ISS 26
FILE LAST UPDATED: 19 Dec 2004 (20041219/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l6
L7 326 L6

=> file registry
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 1.76 318.48

FILE 'REGISTRY' ENTERED AT 13:37:50 ON 20 DEC 2004
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12/20/04

provided by InfoChem.

STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

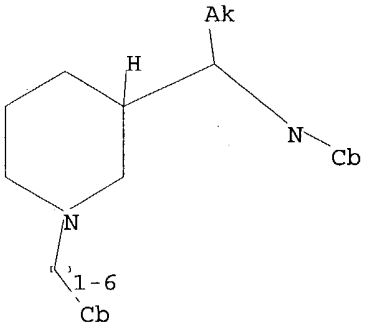
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

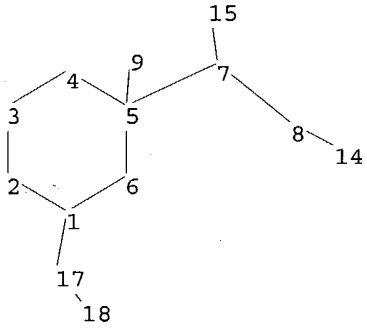
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str





chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18
isolated ring systems :
containing 1 :

G1:H,Ak,Cb

G2:Cb,Ak

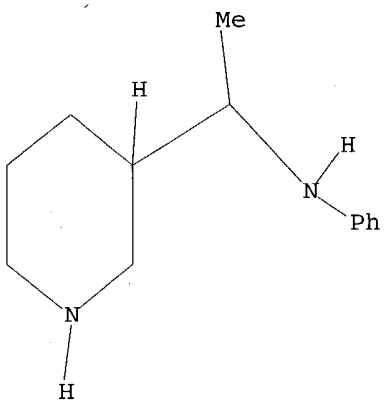
G3:H,Ph,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS 15:CLASS 17:CLASS 18:Atom

12/20/04

L8 STRUCTURE UPLOADED

=> d l8
L8 HAS NO ANSWERS
L8 STR



G1 H,Ak,Cb

G2 Cb,Ak

G3 H,Ph,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l8 ful
FULL SEARCH INITIATED 13:38:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2891 TO ITERATE

100.0% PROCESSED 2891 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L8

=>
=> logoff y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	170.54	489.02

STN INTERNATIONAL LOGOFF AT 13:59:55 ON 20 DEC 2004

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612rxd

10789414

12/20/04

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

```
 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2          "Ask CAS" for self-help around the clock
 NEWS  3  SEP 01  New pricing for the Save Answers for SciFinder Wizard within
                  STN Express with Discover!
 NEWS  4  OCT 28  KOREAPAT now available on STN
 NEWS  5  NOV 30  PHAR reloaded with additional data
 NEWS  6  DEC 01  LISA now available on STN
 NEWS  7  DEC 09  12 databases to be removed from STN on December 31, 2004
 NEWS  8  DEC 15  MEDLINE update schedule for December 2004
 NEWS  9  DEC 17  ELCOM reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  10 DEC 17  COMPUAB reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  11 DEC 17  SOLIDSTATE reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  12 DEC 17  CERAB reloaded; updating to resume; current-awareness
                  alerts (SDIs) affected
 NEWS  13 DEC 17  THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB

 NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:14:56 ON 20 DEC 2004

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:15:05 ON 20 DEC 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

12/20/04

STRUCTURE FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4
DICTIONARY FILE UPDATES: 19 DEC 2004 HIGHEST RN 799762-98-4

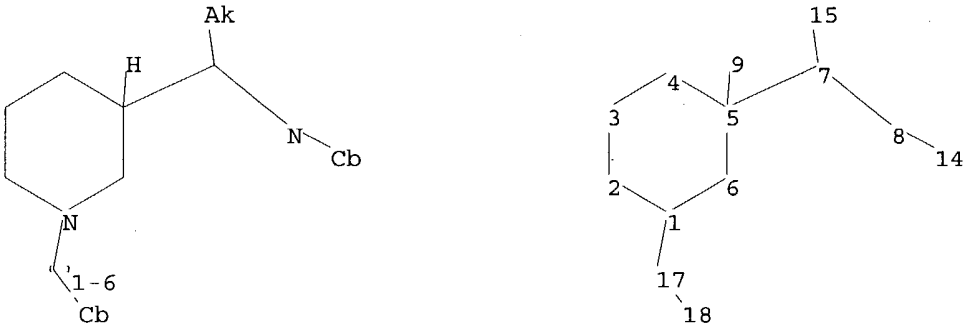
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Stnexp4 corrupted\QUERIES\10789414.str



chain nodes :
7 8 9 14 15 17 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-17 5-7 5-9 7-8 7-15 8-14 17-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-17 2-3 3-4 4-5 5-6 7-8 7-15
exact bonds :
5-7 5-9 8-14 17-18
isolated ring systems :
containing 1 :

G1:H,Ak,Cb

G2:Cb,Ak

G3:H,Ph,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 14:CLASS 15:CLASS 17:CLASS 18:Atom

L1 STRUCTURE UPLOADED

10789414